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MST e-NEWS

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INSIDE

Conradson named AAAS Fellow

Recognized for contributions to physical inorganic chemistry

Steven Conradson (Materials Science in Radiation and Dynamics Extremes, MST-8) has been awarded the distinction of American Association for the Advancement of Science (AAAS) Fellow.

A new fellow in the Chemistry section, Conradson's citation reads: "For distinguished contributions to physical inorganic chemistry with particular emphasis on x-ray absorption spectroscopy and its applications in biology, solid-state physics, and actinide chemistry." The honor is bestowed upon AAAS members by their peers for significant contributions to science and technology.

Photo by Sandra Valdez, IRM-CAS

Conradson obtained a BS in chemistry from San Jose State University and a PhD in physical chemistry from Stanford University. He spent two years at Harvard University on a National Institutes of Heath postdoctoral fellowship. Since joining Los Alamos National Laboratory in 1985, he has participated in multi-institutional projects involving environmental, separations, and

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Revealing the structure behind actinides with remarkable electronic properties

In research featured on the cover of *New Journal of Chemistry*, Steven Conradson (MST-8) and collaborators report the first study of hexacyanoferrate compounds of the light actinides thorium to plutonium since the early investigations during the Manhattan Project some 70 years ago. The study provides a significant advance in our understanding of these compounds, which can be tuned to provide systems that undergo reversible and controlled changes in their physical properties.

Inside front cover of the journal highlights the actinide hexacyanoferrates structural research.

Graphics credit: Christophe den Auwer

The hexacyanometallate family is well known in transition metal chemistry because the possible electronic delocalization along the metal-cyano-metal bond yields remarkable optical or magnetic properties. However, little information on the structural motifs and physical-chemical properties of the actinide analogs exists due to the difficulty in manip-

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Conradson cont.

fundamental actinide chemistry. As project leader of x-ray absorption fine structure spectroscopy, he has worked with a vast number of collaborators from many countries to study radioactive materials at x-ray light sources. In 1993, he pioneered the routine, large-scale application of synchrotron x-ray techniques to determine local structure and chemical speciation in radioactive samples.

Conradson also leads MST-8's Radiation Science, Nuclear Materials and Fuels Experimental Team, which recently reported a number of unique and extreme behaviors in $UO_{2(+x)}$, which is remarkable considering that this industrial chemical is one of the most extensively studied compounds in materials science.

The new class of 388 fellows will be honored in February at the 2014 AAAS Annual Meeting in Chicago.

Technical contact: Steven Conradson

Celebrating service

Congratulations to the following MST Division employees celebrating a service anniversary recently:

Isaac Cordova, MST-6	35 years
Margaret Trujillo, MST-16	35 years
Douglas Hemphill, MST-7	30 years
Kurt Sickafus, MST-8	25 years
Andrew Duffield, MST-6	10 years
John Gibbs, MST-6	5 years

MST e NEWS

Materials Science and Technology

Published by the Experimental Physical Sciences Directorate

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@lanl.gov.

To read past issues, see www.lanl.gov/orgs/mst/mst_enews.shtml.

Los Alamos NATIONAL LABORATORY EST.1943

Actinides cont.

ulating and working with radioactive elements. The properties of the cyano bond make it a very interesting candidate to assess covalent bonding character in the actinide–ligand bond because it forms cyano bridged bimetallic molecular solids and is known to foster electron delocalization. Researchers study covalency within the actinide–ligand bond to predict and control actinide behavior in various domains such as waste management, selective extraction, interaction with the environment, and toxicology.

The researchers synthesized new members of the actinide (IV) hexacyanoferrates with thorium (Th), neptunium (Np), and plutonium (Pu). To cast light on this family of compounds, such as the coordination mode and possible covalency effects, Conradson collaborated with French, German, Russian, and United States researchers in the structural investigation using powder x-ray diffraction, x-ray absorption spectroscopy, and x-ray microscopy for the plutonium adduct. Conradson performed measurements of actinide (IV) hexacyanoferrates for structure determination at the Stanford Synchrotron Radiation Lightsource – SLAC National Accelerator Laboratory.

In the paper, the team described the molecular and crystallographic structure of five representatives (Th^{IV}–Fe^{III}–DMF, Th^{IV}–Fe^{III}–DMF, Th^{IV}–Fe^{II}, Np^{IV}–Fe^{II} and Pu^{IV}–Fe^{II}) of the hexacyanoferrate family with actinide (IV) cations.

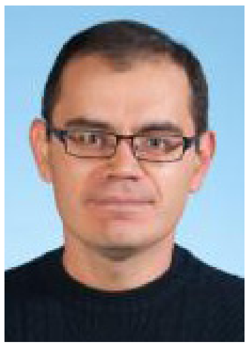
Reference: "Multi-edge X-ray Absorption Spectroscopy of Thorium, Neptunium and Plutonium Hexacyanoferrate Compounds," *New Journal of Chemistry* **37**, 3003 (2013). Researchers include Thomas Dumas (CEA and Helmholtz Zentrum Dresden-Rossendorf), Marie Christine Charbonnel, Clara Fillaux, Philippe Moisy and Sebastien Petit (CEA); Iraida A. Charushnikova (CEA and Russian Academy of Sciences); Steven D. Conradson (MST-8); Christoph Hennig and Andreas C. Scheinost (Helmholtz Zentrum Dresden-Rossendorf); David K. Shuh and Tolek Tyliszczak (Lawrence Berkeley National Laboratory); and Christophe Den Auwer (CEA and Universite de Nice Sophia Antipolis). The DOE Office of Science Heavy Element Chemistry Program sponsored the Los Alamos work, which supports the Lab's Nuclear Deterrence and Energy Security mission areas and the Materials for the Future science pillar.

Technical contact: Steven Conradson

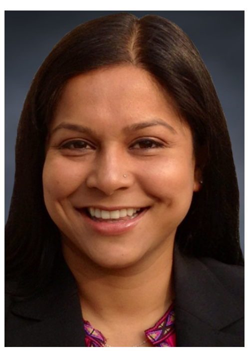
Four MST researchers receive TMS Young Leaders Professional Development Awards

The Minerals, Metals & Materials Society (TMS) has chosen Juan (Pablo) Escobedo-Diaz, Saryu Fensin, Paul Gibbs and Benjamin Morrow to receive the 2014 TMS Young Leaders Professional Development Award.

Established to enhance the professional development of young researchers from TMS's five technical divisions the annual award opens opportunities to participate in TMS activities, attend TMS conferences, network with TMS members and leaders, receive mentoring from TMS division leaders, and serve as judges for division-sponsored student events at the TMS annual meeting



Nominated in the Structural Materials Division, Escobedo-Diaz holds a PhD in materials science and engineering from Washington State University. Following a postdoctoral position at its Institute of Shock Physics, he joined MST-8 as a postdoctoral researcher on the Laboratory Directed Research and Development (LDRD) project "Isolating the Influence of Spatial and Kinetic Effects on Dynamic Damage." His mentors were Ellen Cerreta (MST-8) and Darcie Dennis-Koller (Shock and Detonation Physics, WX-9). Before joining the faculty of the University of New South Wales, Australia, he spent three years at Los Alamos, primarily focused on understanding the linkages between microstructure of metals and dynamic damage evolution, research that was sponsored by LDRD, but led to the development of damage work under Campaign 2. Furthermore, Escobedo-Diaz's portion of this work has resulted in more than 10 peer-reviewed journal papers,



Receiving the award in the Electronic, Magnetic and Photonic Materials Division, Fensin is an expert in molecular dynamics simulations and experiments involving interfaces in mechanical and thermodynamic extremes. Her current work is funded through both an Office of Basic Energy Sciences EFRC, The Center for Materials in Irradiation and Mechanical Extremes (CMIME), and a Campaign 2 project to examine damage in two-phase metals. This work, involves studying the behavior of material microstructure (specifically, single and bi-metal interfaces) on damage nucleation and evolution under dynamic loading conditions. She received her PhD in materials science and engineering from University of California, Davis, joined MST-8 as a postdoctoral researcher in 2010 (mentored by Ellen Cerreta, Steve Valone, and Rusty Gray), and is now a staff member. A TMS member since 2007, she serves on the Mechanical Behavior of Materials, Young Professionals, and Chemistry and Physics of Materials committees.

Nominated in the Materials Processing & Manufacturing Division, Gibbs is a Metallurgy (MST-6) postdoctoral researcher working for Amy Clarke studying the influence of imposed processing variations on solidification microstructure evolution using real-time x-ray and proton imaging, research sponsored by Clarke's Early Career award from the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Gibbs received his PhD in metallurgical and materials engineering from the Colorado School of Mines in 2012. He is the recipient of a 2013 American Iron and Steel Institute Finalist Medal for a paper describing a methodology to produce a family of transformation-induced plasticity steels with desirable austenite stability conditions.

Receiving the award from the Structural Materials Division, Morrow is an MST-8 postdoctoral researcher mentored by Ellen Cerreta. His research is focused on characterization of materials and structure-property relationships in metals. Most recently he is using in situ experiments in a transmission electron microscope (TEM) to directly observe deformation mechanisms and using high-resolution TEM to observe the structure of twin boundaries, research funded by an Office of Basic Energy Sciences project to investigate the constitutive response of hexagonal metals and a Campaign 2 funded program to examine the role of dynamic drive condition on microstructural evolution in zirconium. Morrow received a PhD in materials science and engineering from The Ohio State University in 2011. His thesis work centered on mechanical behavior and characterization of creep mechanisms in zirconium alloys. He has been a member of TMS since 2003 and he serves on the Mechanical Behavior of Materials, Titanium, Young Professionals, and Women in Science committees. His work has also recently been recognized by an honorable mention award, at the Laboratory's 2013 Postdoc Research Day.

TMS is an international professional organization of more than 12,000 members, encompassing the entire range of materials and engineering, from minerals processing and primary metals production to basic research and the advanced applications of materials.

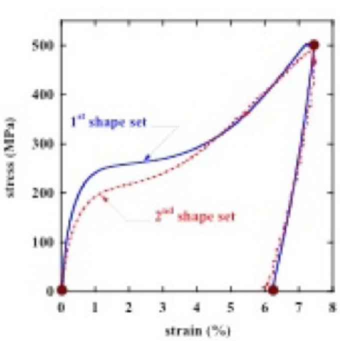
'Shape-setting' mechanics for shape memory alloy actuators

A multi-institutional team of scientists turned to neutron diffraction to identify mechanisms associated with "shape setting" shape memory alloys (SMA). The resulting measurements matched industry standard methods, while simultaneously tracking the underlying microstructure during realistic actuator conditions.

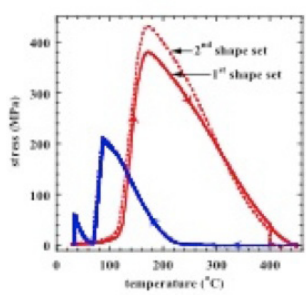
Shape memory alloys are used in applications ranging from medical (stents) to couplings in fighter jets to fluid control military (aerospace couplings) and industrial (automotive transmission fluid control). Shape setting determines the final configuration of shape memory alloy actuators. These data help optimize the load and temperature paths for optimal response, thus expanding the relevance of these materials to large-scale commercial applications.

The experiments performed provide directly measured hard data on the macroscopic and microstructural response of SMA NiTi in situ during typical shape-setting conditions. The information obtained can be used to validate physics-based constitutive models of the SMA effect, furthering the understanding of the process which is required in order to design the load and temperature paths during the shape setting for optimal response of the final SMA product, thus expanding the relevance of these materials to large-scale commercial applications.

While many studies have reported on the microstructure of NiTi and independently on the macroscopic behavior of shape setting NiTi, no experiments have been conducted to mimic the shape-setting process while examining the microstructure and the macroscopic behavior simultaneously. A uniquely suited method for obtaining such concurrent analysis is in situ neutron diffraction. For this work, in situ neutron diffraction experiments were conducted in the Spectrometer for Materials Research at Temperature and Stress (SMARTS) at Los Alamos National Laboratory. SMARTS employs a polychromatic beam from a spallation neutron source with two fixed banks of detectors. Othmane Benefan (NASA) and Doug Nicholson (University of Central Florida) worked with Bjorn Clausen (Lujan Neutron Scattering Center, LANSCE-LC) and Don Brown (MST-8) to obtain the measurements.



Stress vs strain for the first 2 shape-setting cycles for NiTi.



Stress vs temperature for the first 2 shape-setting cycles for NiTi.

The NASA Fundamental Aeronautics Program, Aeronautical Sciences Project funded the work. The Lujan Neutron Scattering Center at LANSCE is funded by DOE Office of Basic Energy Sciences. Reference: "An in situ neutron diffraction study of shape setting shape memory NiTi," *Acta Mater.* **61**, 10 (2013). Researchers include Brown and Clausen, O. Benafan (University of Central Florida/NASA Glenn Research Center); R. Vaidyanathan (University of Central Florida); S.A. Padula II and R.D. Noebe (NASA Glenn Research Center).

Technical contacts: Don Brown and Bjørn Clausen

Laser-induced lensing aids materials evaluation for high-tech refrigerators

Markus Hehlen (Polymers and Coatings, MST-7) and an international team developed a new method for characterizing and optimizing materials for cryogenic optical refrigerators. Optical refrigeration refers to the slowing down of atoms or molecules by the use of a laser whose frequency has been adjusted to remove momentum from the particles. Optical refrigerators operating at cryogenic temperatures are attractive because they can be compact, have no mechanical vibrations or moving parts, and are expected to have high reliability. This emerging technology has possible applications for cooling satellite-based infrared imaging sensors. The journal *Applied Physics Letters* published the research.

Optical refrigeration is achieved by anti-Stokes luminescence, i.e., emission at a mean wavelength shorter than the laser excitation wavelength. Heat (vibrational energy) is removed from the solid and carried away as luminescence. To enable efficient cooling, a material must exhibit certain optical properties, such as a luminescence quantum efficiency close to unity and low background absorption. Undesired non-radiative processes must be minimized.

The team probed thermal and population lensing effects in solid-state optical refrigerators to obtain the sample temperature and other important photo-physical quantities from one measurement. These effects are a direct result of a laser-induced local radial refractive index gradient. They can be detected by observing the time-dependent focusing or defocusing of a coaxial probe beam that passes through the excited volume in the sample. When the excited volume transitions from laser-induced heating to laser induced cooling, the sign of the probe beam time-dependent intensity is inverted due to the change in the sign of the temperature gradient. The scientists introduced a model that includes both laser-induced thermal and population lensing effects. The model describes laser-induced lensing transients and

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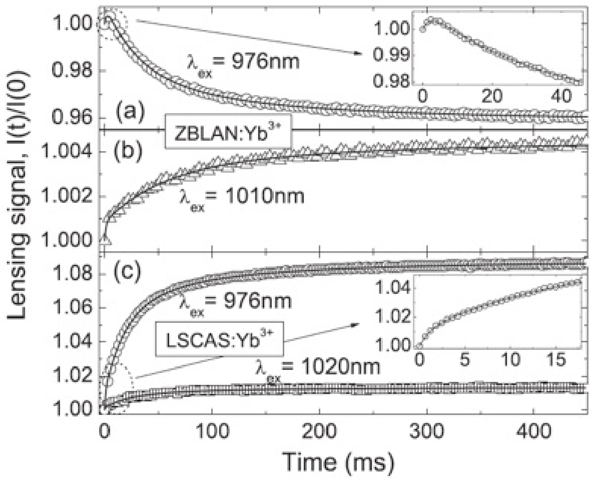


Laser-induced lensing transients measured for Yb^{3+}-doped fluoride (ZBLAN) and aluminosilicate (LSCAS) glasses using different excitation wavelengths (λ_{ex}). Laser excitation of ZBLAN:Yb at 976 nm causes internal heating, inducing a divergent transient lens and resulting in a decaying lensing signal (Panel a). In contrast, using laser excitation at 1010 nm causes internal optical cooling, inducing a convergent transient lens and resulting in an inverted transient (Panel b).

Lensing cont.

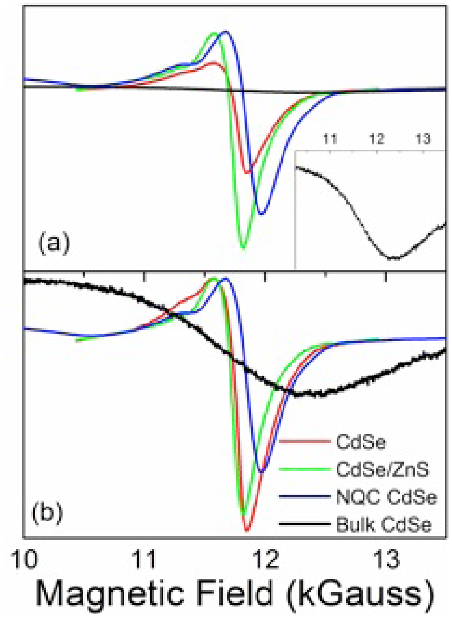
allows for the determination of photo-physical parameters that are important for optical refrigeration. Using time-resolved experiments and their new quantitative method of evaluation, the scientists investigated Yb^{3+}-doped fluoride (ZBLAN) and aluminosilicate (LSCAS) glasses. The team determined the net power, cooling efficiency, and photo-physical properties of the samples. The model revealed thermal and population lensing effects that are induced by laser excitation of Yb^{3+}-doped glasses. The values agreed with previously reported parameters for the fluoride glass ZBLAN. The researchers concluded that aluminosilicate glass is a promising material for high technology refrigeration due to its favorable thermo-optical and mechanical properties. Compared with non-oxide glasses, oxide glasses show greater hardness and thermal conductivity, which are desirable characteristics for laser-cooling applications. The results also demonstrate that this method is a useful tool for the characterization and optimization of optical refrigerator materials.

Reference: “Laser-induced Lensing Effects in Solid-state Optical Refrigerators,” *Applied Physics Letters* **102**, 141910 (2013). Researchers include Markus P. Hehlen (MST-7), J. R. Silva, A. N. Medina, L. C. Malacarne, M. L. Baesso, and N. G. C. Astrath (Universidade Estadual de Maringa Brazil); L. H. C Andrae and S. M. Lima (Universidade Estadual de Mato Grosso do Sul, Brazil); and Y. Guyot (Universite Claude Bernard Lyon, France). The Laboratory Directed Research and Development (LDRD) program funded the LANL portion of the work, which supports the Lab’s Energy Security mission area and the Materials for the Future and Science of Signatures science pillars.

Technical contact: Markus Hehlen

How surface impurities can alter electronic properties in quantum dots

Materials Science and Technology researchers and a collaborator found that impurities on the surface of nanometer-scale cadmium selenide (CdSe) materials can interfere with electronic properties. To their knowledge, this is the first observation of the interaction between conduction electrons in quantum dots and surface impurities. The *Journal of Nanoparticle Research* published the work.



EPR spectra of various CdSe samples. The spectra are (a) measurement at 5 K with the inset showing a magnified view of the bulk CdSe resonance, and (b) normalized spectra at 5K. The legend shown in (b) applies to all of the graphs in this figure.

Quantum dots (QD) are nanoparticles made of semiconductor materials. Those based on CdSe may prove particularly useful in new spin-electronic and spin-photonic devices, detection of single electron spins, and quantum computing architecture. QD also have numerous potential applications as nanoscale semiconductors. Many of these applications fundamentally involve the nature of spin states within the QD.

The scientists examined four types of samples using electron paramagnetic resonance (EPR) spectroscopy: CdSe QDs, CdSe QDs capped by a layer of zinc sulfide (ZnS), non-quantum-confined (NQC, ~15 nm) CdSe particles, and bulk CdSe particles. The team observed unique and complex EPR signals from the CdSe samples. The nitrogen-based impurities on the surface of nanometer-scale CdSe, ZnS coated CdSe, and non-quantum-confined CdSe materials interact with core conduction electrons to yield an anti-ferromagnetic EPR signal at a high resonance field ($g \sim 0.56$). This EPR signal also has a temperature-dependent resonance field that enabled the researchers to determine the coupling strength between the conduction electrons and surface impurities. However, bulk CdSe particles do not show the same anti-ferromagnetic and temperature dependent behaviors. The much larger particle sizes of the bulk materials do not allow significant communication between the CdSe conduction electrons and nitrogen surface im-

continued on next page

Quantum dots cont.

purities. These observations could have consequences for engineering QD systems with tailored electronic and thermal transport properties.

Reference: “Correlated Spin Systems in Undoped CdSe Quantum Dots,” *Journal of Nanoparticle Research* **15**, 1953 (2013). Researchers include Michael W. Blair, Nickolaus A. Smith, Bryan L. Bennett, and Ross E. Muenchausen (MST-7); and Marvin G. Warner (Pacific Northwest Laboratory). The DOE Office of Basic Energy Sciences, Office of Science funded the research, which supports the Lab’s Energy Security mission area and the Materials for the Future science pillar.

Technical contact: Michael Blair

MST engineer featured in workforce diversity magazine

Cindy Sandoval (MST-7) was recently featured in an article about chemical engineers in *Workforce Diversity for Engineering and IT Professionals Magazine*.

Encouraged by a high school counselor to pursue chemical engineering, Sandoval received a bachelor of science degree from Purdue University and a master’s degree in materials science and engineering from National Technological University in 2001.

At Los Alamos National Laboratory, she is an R&D engineer who designs and develops polymeric materials and components for weapons in the U.S. stockpile. Drawing on her understanding of engineering and chemistry, she designs experiments, selects and develops materials, makes prototypes, characterizes and tests materials, analyzes data, and participates in peer reviews.

In the future, Sandoval anticipates more research on nanomaterials as well as additive manufacturing, a method for creating layered materials from three-dimensional simulations. She said she also hopes to spend more time mentoring young scientists in this highly specialized field of materials development for national security applications.

Reference: “Chemical Engineers Solve Problems,” by Lois Vidaver, *Workforce Diversity for Engineering and IT Professionals Magazine*, www.eop.com/wd_article.php?content=ChemicalEngineersSolveProblems. The magazine is free to engineering/IT graduate students and professionals.

Technical contact: Cindy Sandoval

HeadsUP!

How to help an ill or injured co-worker

Entering his office building early one Friday, Tom Archuleta (Plasma Physics, P-24) overheard a co-worker on his Blackberry say he was having difficulty breathing. Archuleta noticed the man’s hand was pressed against his chest. “It looked like he was having a heart attack,” he said. The man, who prefers not to be identified, was sitting on the lobby couch, his face flushed.

Archuleta asked the man a series of questions to determine if he was having a heart attack. Did his arm hurt? Did he have pain or tightness in his chest? The man answered “no,” but said he was struggling for air and his inhaler had not helped. Archuleta instructed another employee, Chris Lovejoy (International Threat Reduction, NEN-3), to call 911. Archuleta, Lovejoy, and NEN-3 Deputy Group Leader Rick Rasmussen stayed by the man’s side until the arrival of paramedics, who administered medication and transported him to the Los Alamos Medical Center emergency room.

“I am feeling pretty good now,” said the man, who had an allergic reaction that September day. “Looking back on the experience, it is very comforting to know that there are good people like Tom who look out for their fellow workers.” He also expressed kind words of appreciation for Lovejoy and Rasmussen. “It felt good to help him,” Archuleta said. “It made my day!” Archuleta is trained in CPR, a requirement of his job, and has used his other life-saving skills outside of work, such as performing the Heimlich maneuver on a young adult choking at a restaurant. “The training that the Lab provides definitely prepared me to help out in those situations,” he said.

Guidelines to follow

1.) Call 911 for assistance if the person’s condition appears to be life threatening (such as a heart attack or severe allergic reaction), if moving the person could be detrimental (such as a neck injury or motor vehicle accident), or if the person requires the expertise and equipment of paramedics.

2.) If a person is unconscious have someone call 911 and start CPR only if you have proper training or find someone who does. Send another person to get an automated external defibrillator (AED). Determine if the person’s breathing and pulse have ceased or seem irregular, then apply the AED immediately. Untreated sudden cardiac arrest causes death in minutes.

3.) Notify the worker’s manager.

4.) Ensure all injuries and illnesses are reported to Occupational Medicine (OM) regardless of where the employee receives medical treatment. Call 667-0660, option 1. If a worker has an open wound in a Radiological Controlled area, remind the worker to report to OM to be examined.

5.) If the injury, illness, or exposure occurs either during off-hours or off-site, contact the on-call OM provider at 667-0660, option 1, for direction on where to report for evaluation and treatment.

For more information on when an employee needs medical care, see int.lanl.gov/employees/health-fitness/occupational-medicine/when-an-employee-needs-medical-care.shtml.

MST reduces electricity usage

The UI-FOD has provided information on electricity usage in ADEPS buildings. As can be seen in the data, ADEPS electricity usage increased 5% from FY12 to FY13, which was due to LANSCE operations. Electrical usage has a significant monetary and environmental impact to our bottom line.

A more detailed look at the data with a focus on MST buildings shows that we reduced our electricity usage in all major facilities including Sigma, the MSC, and TFF. This is excellent news and demonstrates our commitment to the environment and real cost savings.

Please continue to turn off/unplug equipment when not in use, lower room thermostats in the winter at nights and when common areas (conference rooms) are unattended, and turn off office and common area lights if you are the last one out.

A good adage to follow: "If you do it at home (shut off lights and lower thermostats at nights and vacations), then why not do it at work too?"

Thank you for your efforts to reduce electricity usage and please continue your efforts!

Your ADEPS EMS (Environmental Management System) POCs are:

Jim Coy – MST
Susie Duran – MPA
Frances Aull – LANSCE
Steve Glick - Physics

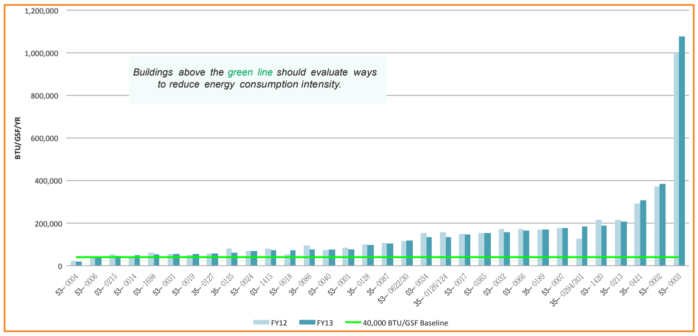
RAD Electricity Report

Fiscal Year Comparison – FY13 vs FY12

Account Number: RAD ADEPS

Billing Period: FY13

ADEPS Building Energy Efficiency – FY12 vs FY13

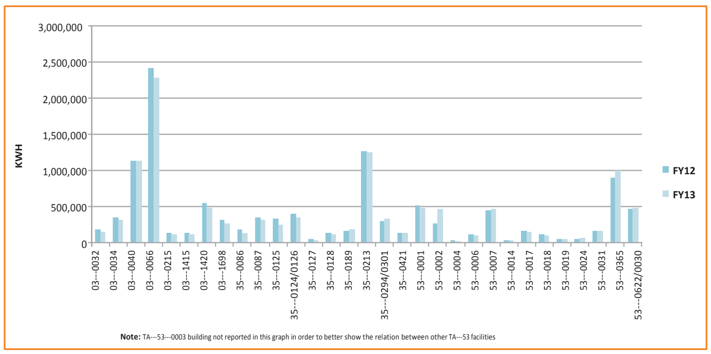


Building Energy Efficiency Comparison

This chart compares the energy efficiency of your RAD's buildings this year with FY12.

*Energy efficiency can be measured by energy intensity—which for an office building is total energy use over time in relation to floor area, counting gas as well as electricity. The **green line** marks DOE's standard for an efficient building: no more than 40,000 Btu/GSF per year or 10,000 Btu/GSF per quarter.*

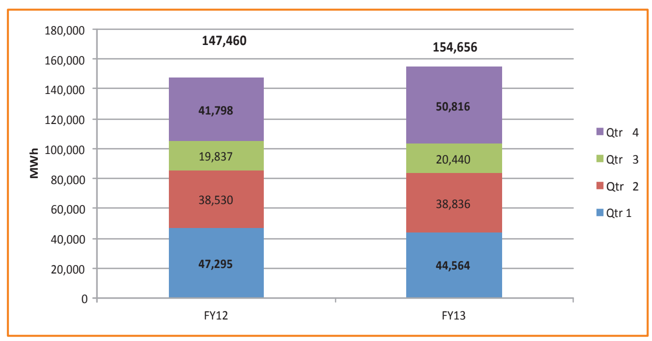
ADEPS Building Electricity Use – Quarter 4 – FY12 vs FY13



Building Electricity Use Comparison

Electrical consumption by your RAD's buildings this quarter compared to the same quarter in FY12

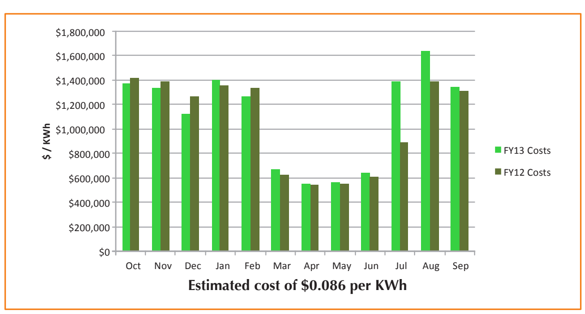
ADEPS Quarterly Electricity Use – FY12 vs FY13



Quarterly Electricity Use Comparison

Quarterly electricity use in megawatt-hours (MWh) for all metered facilities in your RAD during FY12 and FY12

ADEPS Electricity Costs by Month – FY12 vs FY13



Individual Action Steps

- **Unplug unnecessary electronics.**
- **Turn your monitor and the lights off when you leave for a meeting or the day.**
- **Put your computer to sleep or in power down mode when you're not using it.**

We hope this information helps you better understand and make better choices about your RAD's use of electricity.

Questions? Need more information? Go to umetering@lanl.gov